| ESRF | **Experiment title:** Lattice dynamics of Neodymium by grazing-incidence inelastic X-ray scattering and first principles theory | **Experiment number**: HC-864 |
|---|---|---|
| **Beamline**: ID28 | **Date of experiment**: from: 28/02/13 to: 5/03/13 | **Date of report**: 10/08/14 |
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**Report:**

The aim of this experiment was to determine the unknown until now lattice dynamics of Nd by measuring the phonon dispersion branches by grazing-incidence inelastic X-ray scattering (IXS) on an epitaxial Nd film and comparing the experimental data with the results from the ab initio calculations.

Applying the growth conditions described by Soriano et al., [1] single crystalline Nd(0001) film with a thickness of 1.0 μm was grown on a 25 nm thick Nb(110) buffer layer deposited on (11-20)$Al_2O_3$ (A-plane) substrate. After characterization by electron diffraction the film was covered by 10 nm thick Nb layer to protect the reactive Nd metal from oxidation. The film was additionally characterized by XRD that confirmed the formation of high quality *dhcp* Nd(0001). The presence of about 10% *fcc* Nd phase has also been found.

Recently the lattice dynamics of Sm exhibiting the native *9R* (*Sm-type*) structure has been determined by nuclear inelastic scattering and first principles theory and compared with that of the *dhcp* Sm [2]. A remarkable broadening of the longitudinal phonon mode has been observed in experiment that, however, was not found in the calculations. In order to shed more light on this phenomenon, additionally to the *dhcp* Nd, we have measured phonon dispersion relations in *dhcp* Sm film and compared the results to that of Nd. For the purpose of this study a growth procedure for obtaining high-quality epitaxial *dhcp* Sm(0001) on Nb(110) buffered (11-20)$Al_2O_3$ was established. After the growth and characterization the 500 nm thick Sm film was covered by 10 nm Nb and studied by XRD.

The IXS experiment was performed at ID28 of the ESRF with an enery resolution of 2.0 meV. All energy scans were measured at room temperature.

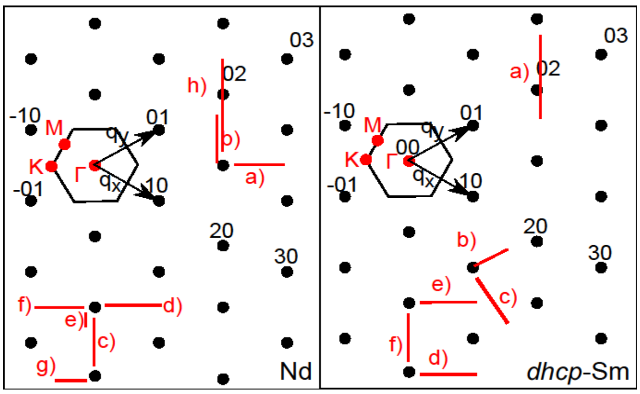


***Fig.1*** *Measured phonon branches for the Nd and Sm films in the $q_x$,$q_y$-projection in the reciprocal space.*

The experiment was performed in grazing incidence geometry that made imposible to map the phonon dispersions along high symmetry directions. All measured branches exhibited an offset in the $q_z$ direction. The measured phonon paths in the reciprocal space projected to the $q_x$-$q_y$-plane for Nd and Sm are shown with solid red/lines in Fig.1. The high symmetry points in $q_x$-$q_y$ plane of the reciprocal space are also indicated.

Selected phonon branches for *dhcp* Nd(0001) and *dhcp* Sm(0001) films compared with the corresponding *ab initio* calculation are shown in Fig. 2 and Fig.3, respectively.

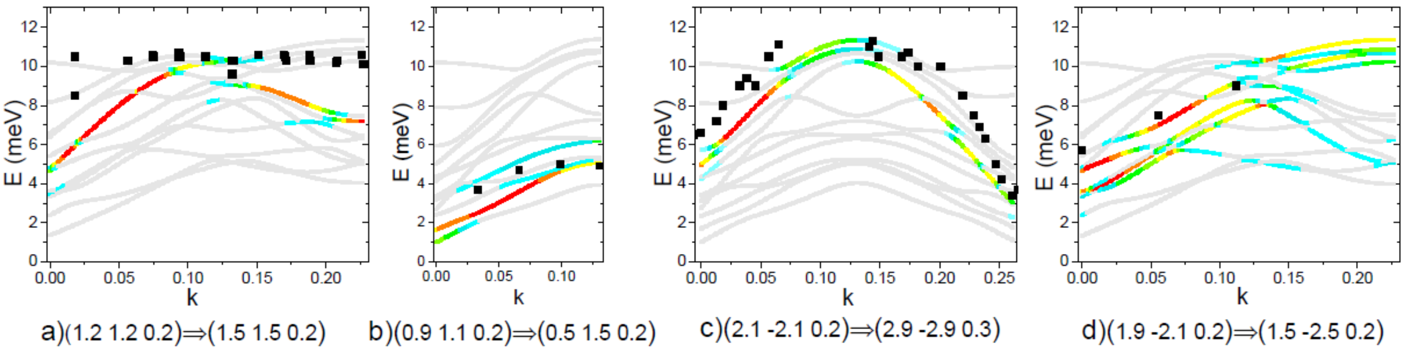


***Fig.2*** *Measured and calculated phonon branches for dhcp Nd (paths a),b),c) and d), Fig1). Black squares correspond to the experimental points and the coloured lines stand for the calculated, projected dispersion relations. Blue stands for the branches with the lowest intensity and red for the branches with the highest intensity. The grey colour depicts branches with lowest intensity that are shown for completeness.*

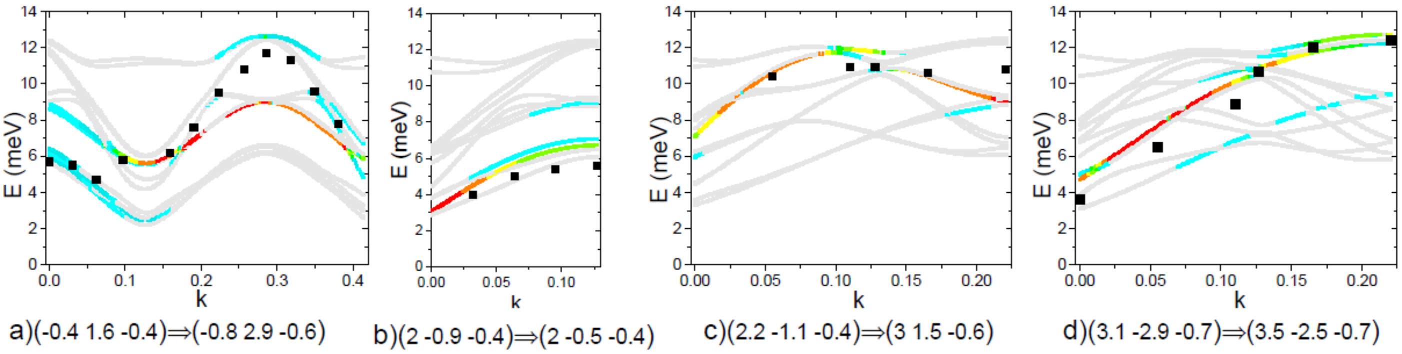


***Fig. 3*** *Measured and calculated branches for dhcp Sm (paths a), b) c) and d), Fig. 1) Black squares correspond to the measured points and the coloured lines stand for the calculated and projected dispersion relations. The colour code is the same as in Fig2.*

The experimental points in Fig 2a) indicate a possible splitting of the optical phonon branch. A similar effect was observed in the phonon density of states of Sm [2]. This splitting was not predicted by the theory and could be attributed to the electron-electron correlations that were not included in the calculations. First-principles calculations applying the LDA+U method that will account for the electron correlations effect are presently on-going.

References:

[1] S. Soriano, K. Dumesnil, C. Dufour, D. Pierre, J. Cryst. Growth 265, 582 (2004)

[2] O. Bauder et. al. PRB 88, 224303 (2013)